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An investigation of Nano-particle Deposition in Cylindrical Tubes under Laminar condition using Lagrangian transport model

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Abstract

Aerosol deposition in cylindrical tubes is a subject of interest to researchers and engineers in many applications of aerosol physics and metrology. Investigation of nano-particles in different aspects such as lungs, upper airways, batteries and vehicle exhaust gases is vital due the smaller size, adverse health effect and higher trouble for trapping than the micro-particles.tt The Lagrangian particle tracking provides an effective method for simulating the deposition of nano-particles as well as micro-particles as it accounts for the particle inertia effect as well as the Brownian excitation. However, using the Lagrangian approach for simulating ultrafine particles has been limited due to computational cost and numerical difficulties.

In this paper, the deposition of nano-particles in cylindrical tubes under laminar condition is studied using the Lagrangian particle tracking method. The commercial Fluent software is used to simulate the fluid flow in the pipes and to study the deposition and dispersion of nano-particles. Different particle diameters as well as different flow rates are examined. The point analysis in a uniform flow is performed for validating the Brownian motion. The results show good agreement between the calculated deposition efficiency and the analytic correlations in the literature. Furthermore, for the nano-particles with the diameter more than 40 nm, the calculated deposition efficiency by the Lagrangian method is less than the analytic correlations based on Eulerian method due to statistical error or the inertia effect.

Keywords: Nano-particle, Two phase flow, Deposition, Lagrangian particle tracking method, Cylindrical tubes

Introduction

Aerosol deposition in cylindrical tubes is a subject of interest by researchers and engineers in many applications of aerosol physics and metrology. Studies on deposition efficiency in lungs, upper airways, batteries and vehicle exhaust gases are some examples of particle deposition in cylindrical tubes. In studying particle deposition in cylindrical tubes, deposition of nano-particles or ultrafine particles (diameter<100nm) are more important among all range of particle diameters. For example, in oral airways, most of particles with the diameter above 1µm are deposited in the nose and respiratory organ walls; however, nano-particles can pass to the lung airways and compromise the human health (Malet, Alloul et al. 2000).

In the literature, numerous studies have developed theoretical expressions for the particle deposition through a smooth tube in laminar flow. Ingham in 1975 and 1991 developed a model for calculating the deposition efficiency in a fully developed flow in cylindrical tube and in the entrance region of a cylindrical tube, respectively (Ingham 1975, Ingham 1991). Cohen and Asgharian in 1990 developed an empirical expression for the deposition efficiency of particles larger than 10nm (Cohen and Asgharian 1990). Most of these studies are used the mass diffusion equation governing the concentration of particles to find an analytic correlation for the deposition efficiency. Therefore, these models often ignore particle inertia effect for aerosols smaller than 200 nm.

In the absence of inertial effects, a highly efficient Eulerian transport model can be applied that treats the particle phase as a dilute chemical species (Longest and Xi 2007). However, the effects of inertia have not been fully quantified for aerosols in the fine and ultrafine ranges (Longest and Xi 2007). Direct Lagrangian particle tracking may provide an effective method for simulating the deposition of nano-particles which can account particle inertia effect. Furthermore, it has the ability to resolve additional body forces that are applicable to each individual particle (Longest and Xi 2007, Tu, Inthavong et al. 2012).

In this study, direct Lagrangian particle tracking method is used to calculate the deposition of nano-particles in cylindrical tubes under the fully developed laminar condition flow. The deposition efficiency is calculated for different flow rates, different tube lengths and different particle diameters.

Mathematical modeling

In this paper, the commercial Ansys-Fluent software is used for solving the governing particle equation of motion. For the fluid flow, the exact solution for laminar pipe flow is used for the fluid velocity as a profile at the inlet of the tube and then the fully developed laminar flow is simulated for the entire cylinder. The exact solution for the laminar flow in the cylinder is a parabolic profile for the velocity which is defined as (Longest and Xi 2007):

$$u(r) = 2u_{in}(1-\frac{r^2}{R^2}) \tag{1}$$

where R is the pipe radius and u_{in} is the inlet velocity.

Then, one-way coupled trajectories of mono-disperse submicron particles ranging in diameter from 5 nm to 100 nm have been calculated based on Lagrangian method by integrating an appropriate form of the particle trajectory equation. In this range of particle diameter, transport of nano-particles is mainly attributed to the Brownian force, therefore, the appropriate equations for spherical particle motion can be expressed as (Wen, Inthavong et al. 2008, Inthavong, Tu et al. 2009):

$$\frac{du_i^p}{dt} = \frac{18\mu}{d_p^2\rho_p C_c}(u_i^g - u_i^p) + F_{Brownian} \tag{2}$$

where u_i^p and u_i^g are the components of the particle and local fluid velocity, respectively. μ is the fluid viscosity and ρ_p is the particle density. C_c is the Cunningham correction factor to Stokes'drag law which can be calculated as (Zamankhan, Ahmadi et al. 2006, Inthavong, Zhang et al. 2011):

$$C_c = 1 + \frac{2\lambda}{d_p}(1.257 + 0.4e^{-(1.1d_p/2\lambda)}) \tag{3}$$

where λ is the mean free path of air which is equal to 65 nm.

The amplitude of the Brownian force is defined as (Wang, Inthavong et al. 2009):

$$F_{Brownian} = \zeta\sqrt{\frac{\pi S_0}{\Delta t}} \tag{4}$$

where ζ is a zero-mean, unit-variance independent Gaussian random number, Δt is the time-step for particle integration and S_0 is a spectral intensity function defined as (Tian and Ahmadi 2007):

$$S_0 = \frac{216 \nu k_B T}{\pi^2 \rho_g d_p^5 \left(\frac{\rho_p}{\rho_g} \right)^2 C_c} \tag{5}$$

T is the absolute temperature of the fluid, ν is the kinematic viscosity, k_B is the Boltzmann constant and ρ_g is the gas density.
Therefore, the Brwonian force can be obtained as (Inthavong, Tu et al. 2009):

$$F_{Brownian} = \frac{\zeta}{m_d} \sqrt{\frac{1}{\tilde{D}} \frac{2 k_B T^2}{\Delta t}} \tag{6}$$

where m_d is the mass of the particle and $\tilde{D}$ is the diffusion coefficient which is determined as (Tu, Inthavong et al. 2012):

$$\tilde{D} = \frac{k_B T C_c}{3 \pi \mu d_p} \tag{7}$$

Geometry and mesh structure

A straight pipe is created in Gambit software in this paper as the studied geometry. The diameter of the pipe is 0.45 cm (Longest and Xi 2007). Two different lengths are considered: 3, 5 cm. The structure of the mesh is an important issue for simulating particle deposition. Fig. 1 displays the created mesh at the inlet of the tube.

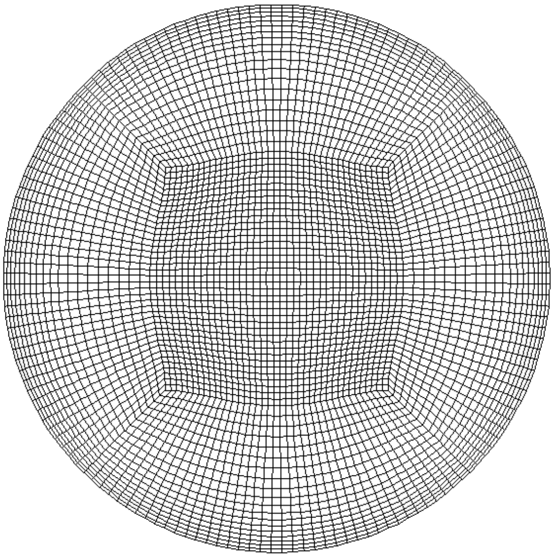

Figure 1. Mesh structure on the pipe inlet

As shown in the figure, dense mesh near the wall is necessary to determine the deposition efficiency correctly (Longest and Vinchurkar 2007). Note that the total number of nodes is almost 900,000.

Boundary conditions

As mentioned before, the deposition efficiency is calculated in a fully developed flow in this paper. Boundary conditions for the particles were set up as a circular particle release entrained in the flow field. Particles were released from 0.01m from the inlet to prevent any spurious data exiting the inlet upon immediate release. In addition, the radial distance at which a particle was located was not less than 0.1 mm away from the wall to eliminate artificial immediate deposition on the walls (Wen, Inthavong et al. 2008). Note that 70000 particles are created randomly in order to have the deposition efficiency independent from the particle number. Furthermore, 10 integration steps for Brownian motion is considered as the time step size (Wen, Inthavong et al. 2008). Note that the considered flow rates are 1 and 2 lit/min.

Results and discussion

Deposition results for the Brownian motion models are first verified by comparing the results with the Ingham equation which proposed an analytic deposition efficiency correlation based on the diffusion parameter. This correlation is defined as (Ingham 1975):

$$DE = 1 - \left(0.819e^{-14.63\Delta} + 0.0976e^{-89.22\Delta} + 0.0325e^{-228\Delta} + 0.0509e^{-125.9\Delta^{2/3}}\right) \tag{8}$$

where Δ is the dimensionless diffusion parameter defined as (Ingham 1975):

$$\Delta = \frac{\tilde{D}L_{pipe}}{4U_{in}R^2} \tag{9}$$

where L_{pipe} is the pipe length.

Fig. 2 displays the deposition efficiency calculated in this paper and by Ingham equation for a pipe with the length of 2 cm and the constant inlet velocity of 1 m/s.

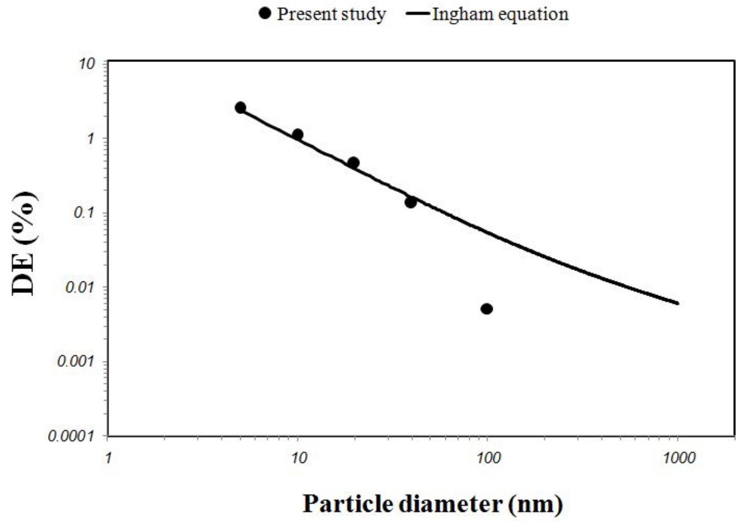

Figure 2. The deposition efficiency for the cylinder with the length of 2cm and the constant inlet velocity of 1m/s

As shown, the results have a good agreement with the Ingham equation. It should be noted that for large particles (40 and 100 nm), due to the inertia effect, the deposition efficiency decreases especially for 100 nm particles (Longest and Xi 2007). As mentioned before, the inertia effect cannot be considered in the Eulerian method or mass diffusion equation and this is another advantage of direct Lagrangian method (Longest and Xi 2007).

Fig. 3 displays the deposition efficiency for both present study and Ingham equation for a 4 cm cylinder with the constant inlet velocity of 1 m/s. As shown, again for 100nm particles, due to the inertia effect, the calculated deposition efficiency is less than the value calculated from Ingham equation.

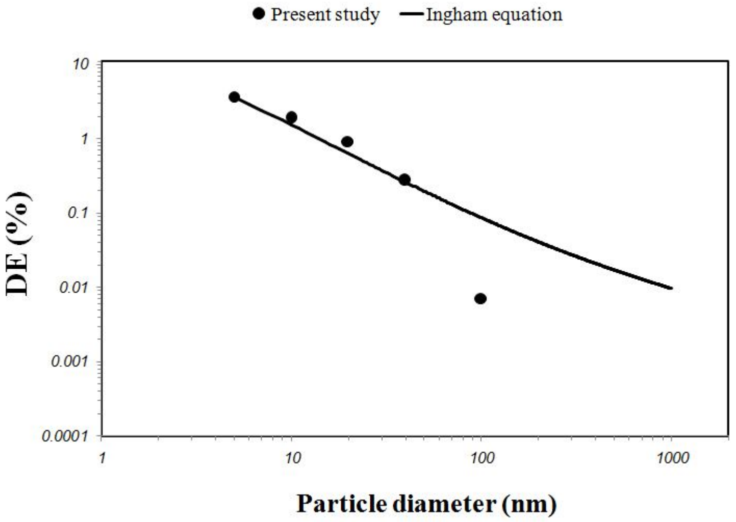

Figure 3. The deposition efficiency for the cylinder with the length of 4cm and the constant inlet velocity of 1m/s

Fig. 4 shows the calculated deposition efficiency in this paper in compare with the Ingham equation for different particle diameter for both tube lengths of 2 and 4 cm for the constant inlet velocity of 2 m/s. As shown, by increasing the inlet velocity, the inertia effect is more effective and for 40 nm particles, the difference between the calculated deposition efficiency and Ingham equation can be seen (Longest and Xi 2007).

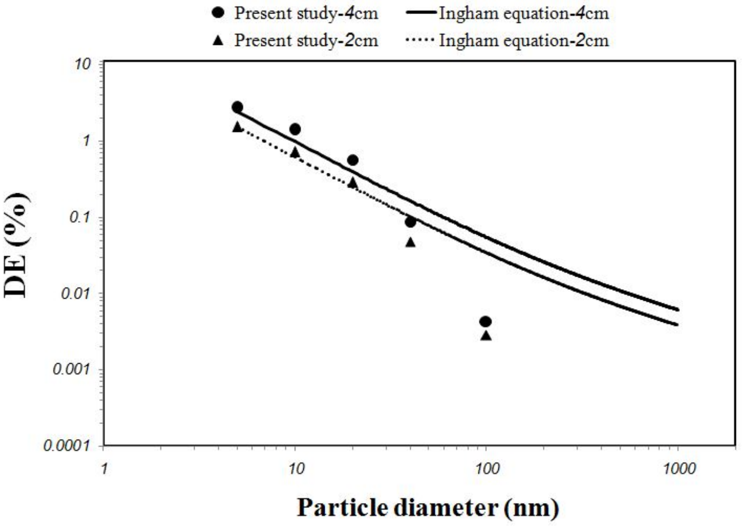

Figure 4. The deposition efficiency for cylinders with the lengths of 2 cm and 4 cm and the constant inlet velocity of 2 m/s

Conclusion

In this paper, the direct Lagrangian particle tracking method was employed to determine the deposition efficiency of nano-particles in cylindrical tubes. Different particle diameters, different flow rates and various pipe lengths were examined. The results showed a good agreement with the existed analytic correlations in the literature. Furthermore, by increasing the particles diameter and inlet velocity, due to the inertia effect, a difference in the calculated deposition efficiency by the Lagrangian method and by the analytic correlation based on diffusion can be seen.

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